In-Class Work: Figures for Scientific Paper & Talk

1. Figure-Requirements: Practice Example

I will walk you through how to use xmgrace to fullfill the following list of requirements for figures for scientific papers and talks. To show you how to do each step in xmgrace we will all start with the same data, the output-files from `md8.py`. I will show you how to make figures as on our webpage (see Guidelines for Main Project).

Copy into your working directory

```
~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/out7_A*.dat
```

Get the first data-set into xmgrace with

```
xmgrace out7_A1.078.dat
```

I will show to you how to get in a second set of data $\omega(t)$ (and how you could also show error bars if available).

Requirements for Figures:

- no title
- axes:
  - label axes (large enough, neat font-tools via clicks and via commands, location of axis label)
  - axis width thick enough
  - number of tick marks large enough
  - tick label size large enough
  - tick marks width and size large enough
  - choose wanted x-range and y-range (main features visible)
- legend (or equivalent with labels) large enough and each set should be labeled (or clear trend of which parameter was varied and in which range) and should not cover data
- label for major parameter large enough (in talk in figure, in paper if not in figure then in figure caption)
- symbols large enough and distinguishable and lines thick enough and distiguishable (keep in mind potential color blind person in audience) and in case of error bars thick enough error bars (labeled: see legend)
- in paper figure caption for each figure

Further xmgrace-tools:

- extra cool fonts: italics, greek, boldface, superscript, shift
- position & size of figure (so that in paper no white frame)
- storing info in file.xmgr (highly recommended)
- printing eps-file (prepare and print; and epstopdf)
- pull in further data-set via block-data
- arrows and labels etc. (drawing objects)
- how to recycle figure via deleting data and replacing with new data or via change of xmgr-file
- symbols: filled and open symbols
- if time: insets
- (not xmgrace but useful: keep logfile for how you made data and where they are)

2. Your Figures

For the next 15 min work on the figures of your main project results. Please ask if you need any further tools, because I could show you several further xmgrace-tools.

In-Class Work: Molecular Dynamics Simulations

10. Forces

We are going to simulate a monatomic liquid. We use the Lennard Potential, that means that the interaction potential V_{ij} of particle i at position $\mathbf{r}_i$ and particle j at position $\mathbf{r}_j$ is

$$V_{ij} = 4\,\epsilon \left(\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right) \tag{5}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. In the simulation we will need forces $\mathbf{F}_i$ on each particle $i = 1, \ldots, N$. We use the relation

$$\mathbf{F}_i = -\nabla_i V = -\nabla_i \sum_{i}^{N-1} \sum_{\substack{j>i \\ j\neq i}}^{N} V_{ij}$$

As preparation for the program determine explicitly the x-component of the force on particle i

$$F_{ix} = \sum_{\substack{j=1 \\ j\neq i}}^{N} -\frac{d}{dx_i} V_{ij}(r_{ij})$$

Upcoming Deadlines:

- April 7: Final Program (graded) $\longrightarrow$ keep working on your project
- April 9, Results section of second paper
- April 9, Results (graded)